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# DEVELOPMENT OF A THREE-DIMENSIONAL COMBUSTOR FLOW ANALYSIS

VOLUME III: USER'S MANUAL FOR THE MINT COMBUSTOR CODE

> United Technologies Research Center East Hartford, Connecticut 06108

> > October 1976

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This report has been reviewed by the Information Office, (ASD/OIP) and its releasable to the National Technical Information Service (NTIS). At NTIS, it will be available to the general public, including foreign nations.

This technical report has been reviewed and is approved for publication.

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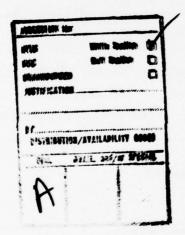
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energy and its dissipation rate is employed via the Prandtl-Kolmogorov hypothesis to determine the turbulent viscosity. The governing equations are solved using the Multidimensional Implicit Nonlinear Time-dependent (MINT) procedure, which employs a unique linearization technique and a Douglas-Gunn alternating-direction-implicit (ADI) scheme. Calculations were made for the flow in a rectangular combustion chamber with a discrete distribution of inlet injection ports. The theoretical analysis and results pertaining to the present study are described in tail in Volumes I and II of the present report. This user's manual provides a general description of the main features of the computer program along with a description of the input variables and a summary of the printed output.





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### INTRODUCTION

Predictions of gas turbine combustor performance and pollutant emission characteristics require modeling procedures possessing a high degree of sophistication. Past attempts at modeling combustion systems have been largely frustrated by the complexity of the coupled hydrodynamic and chemical processes. The difficulty can be largely attributed to the lack of understanding of the flow processes which, through the exchange of heat, mass and momentum, can directly relate to pollutant formation and combustion efficiency. In addition, a reliable calculation procedure must be capable of properly treating the reverse flow recirculation regions occurring in combustion devices. The objective of the present investigation was to extend an existing and relatively efficient United Technologies Research Center three-dimensional Navier-Stokes calculation procedure (Refs. 1 and 2) so that it would be able to compute combusting flows. In particular, the procedure developed solves the timeaveraged three dimensional compressible Navier-Stokes equations including a twoequation transport turbulence model, a pseudo-kinetic hydrocarbon chemistry model, a liquid droplet vaporization model, a single frequency radiation model and a finite rate nitrogen oxide chemistry model. The intent in the development of the flow models described above was to eliminate undue complexity and sophistication, simultaneously providing a reasonably good framework within which refinements could be easily implemented at a future time, if warranted by comparisons with experimental data.

The theoretical analysis pertaining to the present study is described in detail in Volumes I and II of the present report. In view of the preliminary nature of the present work, this user's manual is not intended to be completely comprehensive. A general description of the main features of the computer program is provided along with a description of the input variables and a summary of the printed output.

<sup>1.</sup> Briley, W. R. and H. McDonald: An Implicit Numerical Method for the Multidimensional Compressible Navier-Stokes Equations, United Aircraft Research Laboratories, Report M911363-6, November 1973.

Briley, W. R., H. McDonald, and H. J. Gibeling: Solution of the Multidimensional Compressible Navier-Stokes Equations by a Generalized Implicit Method. United Technologies Research Center, Report R75-911363-15, January 1976.

#### COMPUTER PROGRAM

#### Mode of Operation

The computer program is written to solve the three-dimensional time-averaged compressible Navier-Stokes equations including a two-equation transport turbulence model, a pseudo-kinetic hydrocarbon chemistry model, a liquid droplet vaporization model, and a single frequency radiation transport model. Also, a finite rate nitrogen oxide chemistry model is available using a restart procedure to be described. The numerical procedure solves the time-dependent governing equations beginning with a specified starting solution and appropriate boundary conditions until a steady state solution is achieved.

Several coordinate system options are available in the present computer program. Cartesian coordinates are available for flow problems in rectangular ducts with injection ports on any wall. A generalized axisymmetric orthogonal curvilinear coordinate system is available for flow in axisymmetric combustors with a discrete circumferential distribution of injection ports. However, the computer program has been tested only for cylindrical-polar and cartesian coordinates, and an earlier version of the deck (Refs. 1 and 2) was thoroughly evaluated with cartesian coordinates. The necessary link to generate the metric scale factors for the generalized coordinate system has not been established at this time.

The input data for this program is all in NAMELIST format. Reference values are required for velocity, length, density, temperature, specific heat, dynamic viscosity and molecular weight. Default values for all of these quantities except velocity and length are assumed in the program, and correspond to air at standard conditions. In addition, a nominal nondimensional pressure is required for computation of a pressure difference, which is used in the momentum conservation equations to eliminate truncation errors in pressure gradient terms. The specific heat ratio  $({}_{\rm V})$  is needed to compute a reference frozen sound speed used in calculating a frozen flow Mach number for output only. The units, default values, and Fortran symbols for the reference quantities are given in Table I. Default values for other input variables are given in the input description subsection.

The actual equations to be solved and the appropriate boundary conditions must be specified via input cards to override default values. When a function boundary condition is employed at a wall or port, the desired boundary value of the dependent variable must be specified via the \$BCDATA namelist input unless it is identically zero.

The initial flow field estimate may be obtained in several ways. First, the initial flow field can be generated internally using only inlet profiles and a specified pressure drop from input. Alternatively, the entire starting flow field can be specified via input, if sufficiently smooth consistent flow field data is available. Finally, the initial flow field may be read from a magnetic tape or a disk file generated by a previous run. The latter mode is used for restarting an ongoing solution, and its use is highly recommended to allow checking the solution for errors. At present the restart procedure is required when initiating the kinetic nitrogen oxide chemistry calculation from a converged reacting flow field solution.

Once the initial and boundary data have been specified, the program begins computation. The calculation will proceed for either a specified number of time steps or until the solution changes by less than a user specified tolerance between successive time steps, which ever occurs first.

#### The Calculation Procedure

The MINT (Multidimensional Implicit Nonlinear Time-dependent) Combustor Code combines a main program and a series of subroutines to perform the required calculations. A block diagram of the program is shown in Fig. 1. The main program DAL contains comment and data statements pertaining to the use of the program. Also, DAL calls the main sequence of overlayed subroutines. The input is read, initial parameters are set, and an initial flow field is calculated in subroutine READA and the associated subroutines it calls. If a nitrogen oxide chemistry calculation is being started, subroutine CNOXI is called to initialize all variables necessary for that calculation. Then the execution control subroutine EXEC is called from DAL. Subroutine EXTBV is called from EXEC to initialize the remaining quantities needed to start the calculation, and the initial flow field is printed out by PRNTA. The time step loop is then entered in EXEC and subroutine TSTEP advances the solution through one time step. Various output functions are then performed in EXEC and the next time step is computed. The solution variables are printed out at a specified time step frequency by subroutine PRNTB. The procedure then has completed one time-step calculation. After completion of the specified number of time steps or convergence to a steady solution, the control is returned to the main program DAL where subroutine RESTRT is called to produce a restart dump if desired, and finally subroutine PRNTF is called to obtain the final variables and a limited number of printer plots.

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#### General Features of the Program

The program is written in FORTRAN IV and may require one or more disk files and/or tapes for temporary and permanent data storage.

Type of Fluid

The fluid is a compressible gas with variable thermodynamic properties.

Type of Geometry

Three-dimensional rectangular ducts or axisymmetric geometries with discrete injection ports may be considered (Fig. 2).

Types of Flow

The flow may be turbulent or laminar with heat and mass transfer. Hydrocarbon chemistry, two-phase flows, and flows with recirculation may be treated. Effective exchange coefficients and a two-equation model are employed to model the turbulence. A pseudo-kinetic chemistry and a droplet model are used for the chemical and two-phase flow modeling.

Types of Initial Flow Field Estimate The initial flow field may be read entirely from cards or generated internally by the program (cold start), or be obtained from a magnetic tape or disk file.

Types of Boundary Conditions Function or derivative boundary conditions may be specified for any dependent variable. The time-dependent continuity equation is provided as the boundary condition for the continuity equation at a solid wall. At an inlet port, it is recommended that the density be specified as the continuity equation boundary condition and a second-derivative boundary condition on the pressure should then be employed as the energy equation boundary condition. In any case, the exit port boundary condition for the continuity equation should be a specified static pressure.

Types of Printed Output

An abbreviated summary of the solution is printed out after each time step. In addition, the user may select a time step interval at which a full print of the flow field variables is printed. A full print is also executed after the final time

step of a run along with printer generated time history and spatial plots of selected flow variables.

The IREPUN Option

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Using this option the user may have a restart written on a magnetic tape or a permanent disk file. This file contains sufficient information to start a new run commencing where the previous one ended. The restart file is written after the calculation has proceeded for the user specified a number of time steps, or at a user specified time step interval, or if the program is in danger of exceeding the computer run time limit.

#### Namelist Input Description

Namelist	or
variable	name

Description

\$READ1

Restart option selection

IREST

IREST = 0. A new calculation is being started. Read input from cards. Default.

IREST = 1. Restart option. Read namelist data
from I/O unit number INTAPl and binary (unformatted) array data from unit number INTAPE.

IREST = 4. Restart option. Read namelist data from unit number INTAP1 and formatted array data from unit number INTAPE. In this case, INTAP1 may equal INTAPE.

IREPUN

IREPUN = 0. No restart damp is written during current run.

IREPUN = 1. Write restart dump at time step interval NTREST (see \$READ4 namelist). Namelist data is written onto unit number IØTAP1. Binary (unformatted) array data is written onto unit number IØTAPE.

IREPUN = 4. Same as IREPUN = 1 option except formatted array data is written onto unit number IØTAPE. In this case IØTAP1 may equal IØTAPE.

IØTAPE

Output unit number for dependent variable array restart data. Default is IØTAPE = 10.

INTAPE

Input unit number for dependent variable array restart data. Default is INTAPE = 9.

**IØTAP1** 

Output unit number for namelist restart data. Default is IØTAPl = 20.

INTAPL

Input unit number for namelist restart data. Default is INTAP1 = 19.

Description

NFINP

Not used.

NFØUT

Not used.

\$READ2

Computational grid selection

NUMDX

Number of interior grid points in the X - direction. Two additional boundary points are also required.

NUMDY

Number of interior grid points in the X - direction. Two additional boundary points<sup>2</sup> are also required.

NUMDZ

Number of interior grid points in the X<sub>3</sub> - direction. Two additional boundary points are also required.

XMIN or XGMIN(1)

Nondimensional value of  $X_1$  at boundary number 1 (Fig. 3); identified by index NX1 = 1.

XMAX or XGMAX(1)

Nondimensional value of  $X_1$  at boundary number 2 (Fig. 3); identified by index NX2. XMAX > XMIN.

YMIN or XGMIN(2)

Nondimensional value of  $X_2$  at boundary number 3 (Fig. 3); identified by index NY1 = 1.

YMAX or XGMAX(2)

Nondimensional value of  $X_2$  at boundary number 4 (Fig. 3); identified by index NY2. YMAX > YMIN.

ZMIN or XGMIN(3)

Nondimensional value of  $X_3$  at boundary number 5 (Fig. 4); identified by index NZl = 1.

ZMAX or XGMAX(3)

Nondimensional value of  $X_3$  at boundary number 6 (Fig. 4); identified by index NZ2. ZMAX > ZMIN.

Namelist or variable name	Description
IGRID(I)	Roberts grid transformation sentinel for $X_{I}$ -direction.
	<pre>IGRID(I) = 0. Equally spaced grid points.</pre>
	IGRID(I) = 1. One boundary layer at $XGMIN(I)$ of fractional thickness $GRID(I)$ .
	IGRID(I) = 2. Boundary layers at both $XGMIN(I)$ and $XGMAX(I)$ .
	IGRID(I) = 3. One boundary layer at $XGMAX(I)$ .
GRID(I)	Estimate of boundary layer thickness for Roberts grid transformation in $X_{I}$ - direction; fraction of $XGMAX(I)$ - $XGMIN(I)$ .
IGEOM .	Geometry option sentinel IGEOM = $\pm$ 1. Carstesian coordinate system. IGEOM = $\pm$ 2. Cylindrical polar coordinate system. A negative value of IGEOM results in printout of the metric scale factors and their derivatives. Default value is 1.
TWOD	Logical variable for two-dimensional mode of operation of the MINT code.  TWOD = .FALSE. gives the 3-D mode (default).  TWOD = .TRUE. gives the 2-D mode.
LXTPLT	$X_1$ grid point location for time history printer plots. NX1 $\leq$ LXTPLT $\leq$ NX2.
LYTPLT	$X_2$ grid point location for time history printer plots. NY1 $\leq$ LYTPLT $\leq$ NY2.

Namelist or		
variable name	•	Description
LZTPLT		$X_3$ grid point location for time history printer plots. NZl $\leq$ LZTPLT $\leq$ NZ2.
LXSPLT		X <sub>1</sub> grid point location for spatial printer plots.
LYSPLT		$X_2$ grid point location for spatial printer plots.
LZSPLT		$X_3$ grid point location for spatial printer plots.
LXTPL2		Not used.
LYTPI2		Not used.
LZTPL2		Not used.
CLENG		Reference length (meters). Also appears in \$READ3 namelist.
IDMPX		$X_1$ grid point location for matrix inversion subroutine error check printout (MGAUSS and GAUSS)
IDMPY		X <sub>2</sub> grid point location for matrix inversion printout.
IDMPZ		$X_3$ grid point location for matrix inversion printout.

NUMDX+2.

NUMDY+2.

NXIN

NYIN

NZIN

 $X_1$ -dimension for dynamic storage allocation in the dependent variable array (AC). Default is

 $\rm X_2\text{-}dimension$  for dynamic storage allocation in the dependent variable array (AC). Default is

 $X_3$ -dimension for the dependent variable array. NZIN = NUMDZ+2.

Description

NGPTØT

Total number of grid points for AC array in main

memory; set by program.

**IDGSUB** 

Douglas-Gunn subtraction flag; set by program.

KDIF

Not used.

NPTD

Number of grid points in difference molecule;

must be 3.

BWD

Not used.

KCØEF

Set by program for ADI control.

ISSGEØ

Not used.

INPGEØ

Not used.

ICDC

ICDC = 0 for sector addressable disk usage on

INTVAC.

ICDC = 1 for record addressable disk usage on

CDC.

INOUT

INOUT = 0. All dependent variables stored in

main memory. No mass storage required.

INOUT = 1. Mass storage required for some dependent variables. I/O unit number NUNIT = 11 defined in main program DAL is used for this

purpose.

NWDBLK through

NRECMI

Parameters set by program for control of mass storage input/output of dependent variables

\$READ3

Reference quantities

REY

Reynold's number based on reference quantities;

Re =  $\rho_D U_D L/\mu_D$ . (calculated).

PRNDL

Prandtl number; default Pr = 0.73.

Namelist or	
variable name	Description
SCMDT	Schmidt number; default Sc = 0.73.
PREFF	Effective turbulent Prandtl number; default $Pr_{eff} = 0.90$ .
SCEFF	Effective turbulent Schmidt number; default Sceff = 0.90.
BOLTZ	Boltzmann number; Bo = $\rho_D U_D h_D / q_{R_D}$ (calculated).
WREF	Reference velocity; UD, m/sec.
DENSR	Reference density; default $\rho_D = 1.185 \text{ kg/m}^3$ .
HREF	Reference enthalpy; $h_D = C_{P_D} T_D$ (calculated).
TREF	Reference temperature; default $T_D = 300$ °K.
PREF	Reference pressure; $p_d = 10^3 \rho_D^R g^T D/W_D$ (calculated)
CPREF	Reference specific heat; default c <sub>pD</sub> = 1004.8 joule/kg-°K.
ZREF	Reference reciprocal molecular weight; $Z_D = 10^3/W_D$ moles/kg.
WTREF	Reference molecular weight; default $W_D = 28.966$ gm/mole.
DREF	Reference binary diffusion coefficient; not used at present.
QRREF	Reference radiation energy flux; $q_{R_D}$ , joule/m <sup>2</sup> -sec.
VISCR	Reference dynamic viscosity; default $\mu_D = 1.816$ x $10^{-5}$ kg/m-sec.

variable name	Description
CONDR	Reference thermal conductivity coefficient; $\kappa_{\rm D} = c_{\rm p} \mu_{\rm D}/{\rm Pr}$ (calculated).
SOUND	Reference sound speed; $a_D = (R_g T_D Z_D)^{1/2}$ (calculated).
СМАСН	Reference Mach number, $M = U_D/a_D$ (calculated).
GAMMA	Ratio of specific heats, default $\gamma=1.4$ . Used only in Mach number calculation for output.
RGAS	Universal gas constant, $R_g = 8.3143$ joule/°K-mole.
CLENG	Reference length; L, meters.
PNOM	Nondimensional nominal reference pressure, de- fault PNOM = 1.0.
LAMFLO	Laminar or turbulent flow sentinel.  LAMFLO = 0. Turbulent flow (default).  LAMFLO = 1. Laminar flow.
VISCL	Nondimensional laminar viscosity at standard conditions, VISCL = 1.0.
CTWO	Ratio of second coefficient of viscosity to first coefficient of viscosity; default is 2/3.
AVISC1, AVISC2, AVISC3	Artificial viscosity coefficient for X <sub>1</sub> -, X <sub>2</sub> -, X <sub>3</sub> -directions, respectively. This parameter equals 1/Re <sub>c</sub> where Re <sub>c</sub> is the computational-mesh Reynolds number above which artificial viscosity is required to obtain smooth solutions.
	Default value for each is 0.5.
IHSTAG	<pre>IHSTAG = 0. Static enthalpy option. Default.</pre>
	<pre>IHSTAG = 1. Stagnation enthalpy option.</pre>
	IHSTAG = 2. Constant stagnation enthalpy option.

variable	name
Namelist	or

### Description

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IWFDIF

Velocity wall function differencing flag. Not used when IWVISC = 3.

IWFDIF = 1. Two-point one-sided differencing of  $\partial \widetilde{u}/\partial y$ .

IWFDIF = 2. Central differencing of  $\partial u/\partial y$ . Default.

**IWVISC** 

Turbulent viscosity wall function flag.

IWVISC = 1. Wall viscosity consistent with wall slip velocity.

IWVISC = 2. Match viscosity derivative  $\partial \mu_T / \partial y$  with wall function value.

IWVISC = 3. Match both viscosity derivative  $\partial \mu_T/\partial y$  and velocity derivative  $\partial \widetilde{u}/\partial y$  using generalized wall function formulation (Ref. 3). Default.

YPLØ, YPHI Lower and upper limits of  $y^+$  for which van Driest wall function is employed. Not used when IWUSC = 3. Default YPLO is 2.0, YPHI is 100.0.

CLAMDA

Constant in Lilley's mixing length model (Ref. 3). Default is 0.08.

CWILM

Constant in Williamson's mixing length model (Ref. 3). Default is 0.14.

FLILY

Fraction of maximum velocity which defines shear layer thickness in Lilley's mixing length model. Default is 0.05.

CVK

Von Karman constant. Default is 0.4.

CLW1

Logarithmic wall function constant,  $c_1$  (Ref. 3). Default is 1.0/CVK.

Gibeling, H. J., H. McDonald, and W. R. Briley: Development of a Three-Dimensional Combustor Flow Analysis. AFAPL-TR-75-59, Volume II, October 1976.

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	-	

Namelist or variable name	Description
CLW2	Logarithmic wall function constant, $c_2$ (Ref. 3). Default is 5.1
CTRBMU	Two-equation turbulence model constant, $C_{\mu}$ , (Ref. 3). Default is 0.09.
CTRB1	Two-equation turbulence model constant, $C_1$ , (Ref. 3). Default is 1.55.
CTRB2	Two-equation turbulence model constant, $C_2$ , (Ref. 3). Default is 2.0.
SIGK	Two-equation turbulence model constant, $\sigma_k$ , (Ref. 3). Default is 1.0.
SIGE	Two-equation turbulence model constant, $\sigma_{\rm e}$ , (Ref. 3). Default is 1.3.
FSTKE	Free stream turbulence kinetic energy level; fraction of 0.5 $U_D^2$ . Default is 0.03.
SIGMA	Stefan-Boltzmann constant.
RADLEN	Characteristic frequency-averaged length scale for radiative absorption.
EWRAD	Radiative emissivity of solid walls. Default is 1.0 (black body).
\$READ4	Miscellaneous program control parameters
NT	Number of time steps to be taken. Default is NT = 5.
DT	Initial nondimensional time step; if DT < 0.0 then DT is set to $ DT  * CFL$ . CFL is the explicit stability limit time step.
DTMIN	Minimum nondimensional time step for this run.  If DTMIN < 0.0 then DTMIN is set to DTMIN * CFL.

Description

DTMAX

Maximum nondimensional time step for this run. If DTMAX<0.0, then DTMAX is set to DTMAX \*CFL.

IDTADJ

Time step control sentinel.

IDTADJ = 0. Constant DT is used for the entire
run.

IDTADJ = 1. Time step is adjusted by the factor DELDT based on specified changes PCNT1 and PCNT2. Default.

IDTADJ = 2. Time step is cycled between the specified values DTMIN and DTMAX using an acceleration parameter concept. A sequence of NTSTEP time steps is used under this option.

NTSTEP

Number of time steps for cycling option used for accelerating convergence, see IDTADJ description. Default is NTSTEP = 3.

NTCYST

Time step number during current run at which time step cycling option (IDTADJ = 2) is to be initiated.

SSEPS

Steady-state convergence criteria. Default is SSEPS = 0.001.

DELDT

Factor to increase or decrease time stèp under IDTADJ = 1 option. Default is DEIDT = 1.25.

PCNT1

If maximum relative change in any flow variable is less than PCNT1, the time step is increased to DELDT \* DT (IDTADJ = 1 option). Default is PCNT1 = 0.04.

PCNT2

If maximum relative change in any flow variable is greater than PCNT2, the time step is decreased to DT/DELDT (IDTADJ = 1 option). Default is PCNT2 = 0.06.

Description

TTIME

Nondimensional value of problem time at start of run. For steady computations this value enters only into the pseudo-kinetic hydrocarbon chemistry rate constant.

ESTIME

Estimated computer run time in minutes. If the run time measured from the start of execution of this program exceeds ESTIME at the <u>end</u> of any time step, the program will terminate execution after a normal final print. Default is ESTIME = 600.0 minutes.

IPRINT

Complete flow field printouts are provided every IPRINT time steps. Default is IPRINT = 100

ITEST

Steady state test is performed every ITEST time steps. Default is ITEST = 1.

IPLOT

Not used at present.

ITPLT

Number of time steps for which selected time plot data are saved on restart. Set by program.

NTREST

Time step interval at which restart dumps are taken. See IREPUN description under \$READ1 namelist.

IDUMP1

Supplementary print flag.

IDUMP1 = 1. Print initial flow field.

IDUMP1 = 2. No initial printout.

IDUMP1 =-1. Print initial flow field and solution variables at the end of each ADI step for the first time step.

IDUMP1 = 0. Print solution variables at end of each ADI step for first time step.

Default is IDUMP1 = 1.

variable	
Namelist	or

#### Description

MGPRNT

Matrix inversion routine error-check printout is provided every MGPRNT time steps. This print is automatically provided at the first time step. Default is MGPRNT = NT.

NAMLST

Sentinel for optional namelist input in subroutine BVIV. NAMLST = 0: No additional input read.

TEXIT

If the computer run time remaining at the end of any time step is less than TEXIT, the program will terminate execution after a normal final print. Default is TEXIT = 20.0 seconds.

TSTOP

If the nondimensional problem time TTIME exceeds TSTOP, the program will terminate execution in the normal manner. Default is TSTOP =  $10^{10}$ .

MEQS

The total number of equations to be solved during the flow field calculation procedure (NOX chemistry is not included). The actual equations are specified via the IEQNUM array.

MCPLD

The total number of equations to be solved coupled during each ADI sweep. Used only when NPADI = 1.

NEQN(IP, IADI)

The number of coupled equations to be solved during sequence number IP of sweep IADI.

NEQN(IP+1, IADI)

The number of decoupled equations to be solved during sequence number IP of sweep IADI.

NPADI

The number of sequences of coupled and decoupled equations to be solved during each ADI step.

<sup>&</sup>quot;The notation "coupled" and "decoupled" is used here to indicate coupling between the finite difference equations during any ADI step.

Description

INPEQS

Not used.

IEQNUM(J)

Array containing the external equation numbers (see Table II) of the equations to be solved;  $1 \le J \le MEQS$ .

IVARNO(I)

The index of the dependent variable associated with external equation I = IEQNUM(J). See Table II.

ISOLVE(I)

Flag which specifies if the external equation I = IEQNUM(J) is to be solved during the present run, or at a later time via a restart.

ISOLVE(I) = 0. Do not solve equation.

ISOLVE(I) = 1. Solve equation.

ISOLVE(I)  $\geq$  2. Solve equation at a later time, by specifying ISOLVE = 1 in the restart mode. Devault values are given in Table III.

ICPLD(I,IADI)

Coupled equation sentinel for external equation number I on ADI sweep IADI (IADI = 1,2,3). Default values are set in main program DAL. See Table III. The meaning of these values is as follows, where IP = ICPLD(I,IADI).

1 ≤ IP ≤ 10. Equation number I is coupled\* during sequence number IP of sweep IADI.

11 ≤ IP ≤ 20. Equation number I is decoupled\*
during sequence number (IP - 10) of sweep IADI.

21  $\leq$  IP  $\leq$  30. Equation number I is independent of flow field during sequence number (IP - 20) of sweep IADI.

IP = 0. Equation number I is not solved during
sweep IADI.

<sup>\*</sup> See previous footnote.

Namelist or	
variable name	Description
JEQN(I,IADI)	External equation number of the Ith equation which is solved during sweep IADI. Set by program.
JVAR(I,IADI)	Variable number associated with the Ith equation which is solved during sweep IADI. Set by program.
NVDMP	The number of dependent variables in the AC array to be written on the restart dump. Only a single time level is written for these variables. Default is NVDMP = MEQS.
NVDMP1, NVDMP2	Indices for dumping the remainder of AC array required for a restart. Set by program.  NVDMP1 = NVDMP + 1; NVDMP2 = last variable index being used by program.

The following variables are integer indices used in referencing the correct component of the AC array in the program. These variables are stored at two time levels.

U	u - velocity component index
V	v - velocity component index
W	w - velocity component index
R	Density index
Н	Stagnation or static enthalpy index
MF	Unburned fuel mass fraction $(m_1)$ index
MFP	Mixture fraction (*) index
TKE	Turbulence kinetic energy index
TED	Turbulence kinetic energy dissipation rate index

Namelist or Variable name	Description
VS	Effective viscosity index
NO	Nitrogen oxide mass fraction index
NPARTI	Lower particle fraction equation number
NPART2	Upper particle fraction equation number
The following variables are i stored in the AC array at onl	nteger indices used in referencing quantities y a single time level.
T, TL	Temperature index
ME, MEL	Equilibrium hydrocarbon fuel mass fraction $(m_{le})$ index
CH,CHL	Reciprocal specific heat index $(c_H = 1/c_p)$
ZN,ZNL	Reciprocal molecular weight (Z) index
D,DL	Velocity devergence index
P,PL	Static pressure difference (p-p <sub>nom</sub> ) index
VAP,VAPL	Droplet vaporization source term index
CK1,CK1L	Hydrocarbon chemistry function index
CK2,CK2L	Hydrocarbon chemistry function index

CKM, CKML

CKH, CKHL

CKP, CKPL

NO1, NO1L

NO2, NO2L

Hydrocarbon chemistry function index

Hydrocarbon chemistry function index

Hydrocarbon chemistry function index

Nitrogen oxide chemistry function index

Nitrogen oxide chemistry function index

Description

NO3,NO3L

Nitrogen oxide chemistry function index

NO4, NO4L

Nitrogen oxide chemistry function index

DLIMIT

Not used

IDIFF(IADI, IEQ)

Sentinel for optional nonlinear differencing formulas.

IDIFF = 0. Employ conventional central difference formulas. Default.

IDIFF = 1. Employ nonlinear difference formulas for ADI sweep number IADI in equation number IEQ.

NCOMP

Number of components for multicomponent flow.

NCOMP = 1. Single component flow of air.

NCOMP = 2. Two-component flow of methane and air (default). Other species may be treated by reading in the appropriate thermodynamic data in JANNAF format into the CG array in the \$CHEMD namelist.

NPART

Number of particle fraction classes for droplet vaporization model. NPART ≤ 4. Default is NPART = 0, which means that droplet vaporization will not be considered. Note that program dimension NVAR in the AC array must be increased by NPART for storage of droplet particle fractions.

PSTAT1

Average nondimensional inlet static pressure.

Default is PSTAT1 = 1.0.

RH01

Not used.

**PDROP** 

Pressure drop parameter. The specified exit static pressure is set to PSTAT = PDROP \* PSTAT1.

Namelist or variable name Description Not used. RMF LW1 Not used. CMFLW(J) Pressure differencing parameter. **IPGRAD** IPGRAD = 0. Central differencing of pressure in all coordinate directions. Default. IPGRAD = 1. One-sided differencing in  $X_1$ and X2 directions. IPGRAD = 2. Nonlinear differencing in  $X_1$  and X2 directions. Optional print control flag. LZPRNT(LZ) LZPRNT = 0. Suppress all flow field printout at axial station number LZ. LZPRNT = 1. Normal flow field printout at axial station LZ. Default is 1. Optional print control flag for dependent vari-IVARPR(IV) able number IV. (Table II). IVARPR = 0. Suppress printout of variable IV. IVARPR = 1. Normal printout of variable IV. Default. \$READ5 Boundary conditions and wall-port specification IBOUND (IBC) Boundary-type indicator for surface IBC (See Figs. 3,4). See Table V for default values. IBOUND = 1. Inlet or exit plane (no walls).

\*A wall-function surface is a wall at which a slip velocity is determined using the law-of-the-wall.

IBOUND = 2. Plane of symmetry.
IBOUND = 3. Free surface.

IBOUND = 6. No slip wall.

IBOUND = 4. Wall-function surface\*.

IBOUND = 5. Wall-function surface\* with ports.

#### Description

# IEQBC(IBC,I)

Boundary condition specification for external equation number I at surface IBC (See Figs. 3,4). See Table IV for default values.

Standard boundary conditions (no testing for ports):

TEQBC = 1. Function boundary condition (dependent variable only).

IEQBC = 2. First derivative of dependent variable equals 0.0.

TEQBC = 3. Second derivative of dependent variable equals 0.0.

Special boundary conditions (test for ports if
IBOUND(IBC) = 5):

Continuity equation (I = 4)

TEQBC = 4. At a wall, apply time-dependent continuity equation. At a port, specify density or apply a pressure boundary condition, as determined by ICONBC(IBC), see below.

#### Energy equation (I = 5)

IEQBC  $\geq$  4. At a wall, apply adiabatic wall condition.

IEQBC = 4. At the inlet, specify static temperature (see initial flow field input description). Cannot be used when density is specified at the inlet.

IEQBC = 5. Not used.

IEQBC = 6.  $\partial p/\partial n = 0$  where p is static pressure and n is normal to surface IBC.

IEQBC = 7.  $\partial^2 p/\partial n^2 = 0$  (recommended).

Momentum equations (I = 1,2,3) wall boundary conditions:

IEQBC = 4. Wall function boundary condition (no ports permitted).

IEQBC ≥ 5. Wall function boundary condition at wall grid points.

IEQBC(IBC,I)
continued

### Description

Momentum equations (I = 1,2,3) and species equations (I = 6 to 12) port boundary conditions. IEQBC = 5. Function boundary condition, i.e., specified velocity, mass fraction or particle fraction profiles. IEQBC = 6.  $\partial \phi_{\rm T}/\partial n = 0$  IEQBC = 7.  $\partial^2 \phi_{\rm T}/\partial n^2 = 0$  Species equations (I = 6 to 12) wall boundary condition IEQBC  $\geq 4$ . First derivative of mass fraction or particle fraction equals zero.

### Radiation transport equations (I = 13 to 15)

IEQBC = 4. At a wall, the specified wall temperature  $(T_w)$  boundary condition is applied. At present  $T_w = 300^{\circ} K$  is employed and the wall emissivity is taken as  $\epsilon_w = 1$ . At a port, outgoing radiation escapes and the appropriate boundary condition requires a specified incoming radiative flux,  $q_{in}$ . At present  $q_{in} = 0.0$  is employed.

Turbulence kinetic energy equation (I = 16) IEQBC = 4. At a wall, linearly extrapolate k from interior points using  $\partial^2 k/\partial n^2 = 0$ . IEQBC = 5. Inflow port designation, specified k. IEQBC = 7. Outflow port designation,  $\partial^2 k/\partial n^2 = 0$ .

# Turbulence kinetic energy dissipation rate equation (I = 17)

IEQBC ≥ 4. At a wall, € is specified consistent with wall function formulation at one grid point away from wall.

IEQBC = 5. Inflow port designation, specified  $\varepsilon$ . IEQBC = 7. Outflow port designation,  $\partial^2 \varepsilon / \partial n^2 = 0$ .

### Description

ICONBC (IBC)

Continuity equation port boundary condition indicator for surface IBC. See Table IV.

ICONBC = 1. Specified density at port (recommended at inlet or injection ports).

ICONBC = 2. Specified static pressure at port (recommended at exit port)

ICONBC = 3. Specified stagnation pressure at port.

ICONBC = 4. Specified  $\partial p/\partial n$  at port. ICONBC = 5.  $\partial p/\partial n = 0.0$  at port. ICONBC = 6.  $\partial^2 p/\partial n^2 = 0.0$  at port.

NPORTS

Total number of ports on all boundaries. NPORTS  $\leq 6$ .

LCPORT(NP)

Must be set equal to the surface number IBC (Figs. 3 and 4) containing port number NP.

IPOR1(ILU, IG2, NP)

Port coordinate specification. When ILU equals 1 (or 2) IPOR1 designates the lower (or upper) grid point number (for port number NP) in the  $X_1^*$  - coordinate direction at grid point number IG2 in the  $X_2^*$  - coordinate direction. See footnote below.

IPOR2(ILU, IG1, NP)

Port coordinate specification. When ILU equals 1 (or 2) IPOR2 designates the lower (or upper) grid point number (for port number NP) in the  $X_2^*$  - coordinate direction at grid point number IGl in the  $X_1^*$  - coordinate direction. See footnote below. The specification of IPOR2 must be consistent with that of IPOR1, and it is required to define a general port geometry and to avoid excessive internal testing in the program.

Note on port coordinate specification. The actual coordinate directions corresponding to  $X_1^*$  and  $X_2^*$  are determined by the surface (IBC) which contains the port NP, as indicated in the following table:

IBC	x,*	x*
1,2	X <sub>2</sub>	X <sup>3</sup>
3,4	x	x <sub>3</sub>
5,6	x <sub>1</sub>	x <sub>2</sub>

Also, the grid point numbers specified in the IPOR1 and IPOR2 arrays are assumed to coincide with the wall grid point closest to the port under consideration. If the computational boundary coincides with a line of symmetry through the port, then the values of IPOR1 (or IPOR2) defining that port boundary must be set to zero.

4	CHEMI	
4.	CHIMI	
Ψ	CILLET	ı

#### **ICHEMR**

JCHEM

ATC, ATH

OXMF

TFLOOR

### Chemistry and droplet data

Hyrdocarbon chemistry sentinel
ICHEMR = -1. No chemical reactions,
variable specific heat (cp) using JANNAF
data.

ICHEMR = 0. No chemical reactions, constant specific heat  $(c_p)$ . See CCP input description below.

ICHEMR = 1. Pseudo-kinetic hydrocarbon chemistry, variable specific heats ( $c_{p_i}$ ) using JANNAF data.

Chemistry flag set in subroutine TEMPN

Hydrocarbon fuel specification,  $C_{nmm}H$ , where n = ATC, m = ATH. Defaults are ATC = 1.0, ATH = 4.0 (methane).

Mass fraction of oxygen  $(O_2)$  in the oxidizer (normally air). OXMF = 0.2322 for air.

Nondimensional minimum temperature permitted with chemistry. Default is TFLOOR = 300°K/TREF.

Description

CHFM(J)

Heat of formation of component J (kcal/mole)

J = 1: methane (CH<sub>4</sub>), CHFM = 17.895 kcal/mole.

J = 2: air, CHFM = 0.0.

CMW(J)

Molecular weight of component J (gm/mole).

J = 1: methane, CMW = 16.043.

J = 2: air, CMW = 28.966.

CMWINV(J)

Inverse of CMW(J), calculated.

CCP(J)

Specific heat of component J (joule/kg-°K) for ICHEMR = 0 option.

J = 1: methane, CCP = 1884.0 joule/kg-°K.

J = 2: air, CCP = 1004.8 joule/kg-°K.

IFUEL

Fuel species index for JANNAF tabular data. Default is IFUEL = 12, see BLOCK DATA subprogram (CHEMDATA) and CG description below.

ISPEC

Total number of species in the JANNAF table (CG array, see below). ISPEC = 15.

TCHEM1, TCHEM2, TCHEM3 TCHEM1 is the nondimensional start time for pseudo-kinetic hydrocarbon chemistry. If TCHEM1 < TTIME < TCHEM2, use TSCAL1 as the HC chemistry kinetic time scale. If TCHEM2 < TTIME < TCHEM3, decrease the kinetic time scale from TSCAL1 to TSCAL2 using a cosine function of time. If TTIME > TCHEM3, use TSCAL2 as the HC chemistry kinetic time scale.

TSCALL, TSCAL2

Nondimensional time scales for pseudokinetic HC chemistry calculation.

Description

IRCON

Rate constant (or time scale) control sentinel for pseudo-kinetic HC chemistry calculation. Determines the type of ignition delay used in the HC chemistry calculation.

IRCON = 0. No delay; i.e., rate constant
independent of distance from inlet port.

IRCON = 1. Linear variation of rate constant  $r_c$  as a function of distance from inlet port, where (TSCALL)<sup>-1</sup>  $\leq r_c \leq (\text{TSCAL2})^{-1}$  for ZMNRAT  $\leq X_2 \leq \text{ZMXRAT}$ .

IRCON = 2. Quadratic variation of rate constant as a function of distance from inlet port.

ZMNRAT

Nondimensional value of  $X_3$ -coordinate such that the rate constant equals (TSCALL)<sup>-1</sup> in the range ZMIN  $\leq X_3 \leq$  ZMNRAT. Default is ZMNRAT = Z(3).

ZMXRAT

Nondimensional value of  $X_3$ -coordinate at which the rate constant reaches the maximum value (TSCAI2)<sup>-1</sup>. See IRCON discussion above. Default is ZMXRAT = ZMAX.

LZRAT1

Optional. If specified then ZMNRAT is set equal to Z(LZRAT1).

LZRAT2

Optional. If specified then ZMXRAT is set equal to Z(LZRAT2).

FRATE

Rate constant multiplier. Default is
FRATE = 1.0.

EPST

Not used at present.

ITERT

Not used at present.

NOX

NTNOX

NOXUN

NOREST

#### Description

Nitrogen oxide chemistry sentinel.

NOX = 0. Do not solve NO chemistry equation.

NOX = 1. Solve NO chemistry equation after convergence of flow field solution. This option is not operational.

NOX = 2. Solve NO chemistry equation using flow field obtained from a restart dump.

Number of time steps for NO chemistry calculation. Overrides input value of NT.

Output unit number for partial equilibrium mole fraction data calculated during the nitric oxide chemistry initialization procedure in subroutine CNOXI. The partial equilibrium calculation is fairly time consuming, so it is desirable to save the necessary mole fractions on a disk or tape file. Default is NOXUN = 21.

Nitric oxide chemistry restart option. See NOXUN above.

NOREST = 0. Do not write partial equilibrium mole fraction data on unit NOXUN.

NOREST = 1. Write partial equilibrium mole fraction data on unit NOXUN (default).

NOREST = 2. Read partial equilibrium mole fraction data from unit NOXUN.

#### Description

FNOXST

The initial guess for nitric oxide mass fraction is set equal to FNOXST times the value obtained from the partial equilibrium calculation. Default is FNOXST = 0.01.

ANOX(J), BNOX(J),

PNOX(J),

Chemical rate constants for extended Zeldovich nitric oxide reaction mechanism. An Arrenhius form is assumed:  $k_j = A_j T^p j$  exp  $(-B_j/RT)$ . See Table V for values and units.

The following input parameters pertain to the partial equilibrium calculation (subrouting EQUIL) needed for the nitric oxide chemistry initialization procedure (subroutine CNOXI).

FAMAX

Maximum fuel-to-air mass ratio for which the equilibrium calculation will be performed. Default is FAMAX =  $1.0 \times 10^{14}$ .

EPSEQM

Convergence criterion for equilibrium

Newton-Raphson iteration procedure (subroutine EQUIL). Default is EPSEQM = 1.0
x 10<sup>-5</sup>

EPSEQT

Convergence criterion for initial temperature guess (needed by EQUIL) iteration procedure (subroutine SET1). Default is EPSEQT = 1.0x10<sup>-5</sup>.

Description

TMIN

Minimum temperature allowed during EQUIL iteration. Default is TMIN = 290°K.

XAMT

Maximum temperature allowed during EQUIL iteration. Default is TMAX = 6000°K.

ICEQMX

Maximum number of iterations for EQUIL iteration procedure. Default is ICEQMX

= 25.

XAMTW.

Maximum number of iterations for SET1 iteration procedure. Default is NTMAX = 10.

The following input parameters pertain to the droplet vaporization model.

RDROP(J)

Discrete droplet radii (meters) for the particle fraction classes (see Fig. 5);  $1 \le J \le NPART + 1$  and RDROP(K) >RDROP(K+1) is required. Default values are 1.25x10<sup>-4</sup>, 1.0x10<sup>-4</sup>, 0.75x10<sup>-4</sup>, 0.5x10-4, 0.25x10-4m, respectively.

RHODR

Droplet (liquid) density, a constant. Default is RHODR = 640.7 kg/m<sup>3</sup> (liquid CHL).

HDVAP

Heat of vaporization of the liquid droplets. Default is HDVAP = 0.31966x106 joule/kg (liquid CH4).

HDCOMB

Heat of reaction for stoichiometric combustion of the fuel with  $O_2$ . Default is HDCOMB =  $50.2 \times 10^6$  joule/kg ( $CH_{l_4}$ ).

RSTC

Ratio of fuel mass to oxygen mass for the stoichiometric combustion reaction. Default is RSTC = 0.25 (CH<sub>L</sub> + 20<sub>2</sub> -CO2 + 2H2O).

Description

RHDVAP

Inverse of HDVAP. Calculated.

CRDR1(J),
CRDR2(J)

Calculated functions of the radii RDROP:  $1 \le J \le NPART + 1$ .

The following input arrays contain the chemical species thermodynamic data. Polynomial fits to the JANNAF data have been made over two temperature ranges (300 - 1400°K and 1400-6000°K). Seven polynomial coefficients are stored for each required species (see Table VI) for each temperature range.

CG(I,IS)

Polynomial coefficients for species number IS. Temperature range 1400 - 6000°K, 1  $\leq$  I  $\leq$  7; temperature range 300 - 1400°K, 8  $\leq$  I  $\leq$  14. The format of CG is implied by the following non-dimensional polynomial relationships, with C<sub>I</sub> designating CG(I,IS) or CG(I+7,IS) for the two temperature ranges considered:

sidered:  

$$\frac{C_p}{R} = C_1 + C_2T + C_3T^2 + C_4T^3 + C_5T^4$$
  
 $\frac{H}{RT} = C_1 + \frac{C_2T}{2} + \frac{C_3T^2}{3} + \frac{C_4T^3}{4} + \frac{C_5T^4}{5} + \frac{C_6}{T}$ 

where R is the universal gas constant, and  $C_p$  and H are the molar specific heat and molar enthalpy, respectively. The temperature T is in degrees Kelvin, which implies the units for the coefficients  $C_I$  (I = 1 to 6). The coefficient  $C_I$  is not required in the present analysis?

Molecular weight of species IS, gm/mole. See Table VI.

Nondimensional polynomial coefficients for fuel (J = 1) and air (J = 2) calculated from CG data.

SMW(IS)

ACP(I,J)

SHFM(IS)

BETA(IS, JE)

# Description

Nondimensional heat of formation of species IS calculated from CG data.

Atomic stoichiometric coefficients: the number of gm-atoms of element JE per gm-mole of species IS. See Table VII.

### Namelist Input For Initial Flow Field

This input is read in subroutine FLWFLD only if IREST = 0, and following the previous namelist \$READl through \$CHEMD. Namelist \$BOUND is read once, and then namelist \$BCDATA is read at each  $X_3$  - coordinate location (see Fig. 4) for which LZREAD(LZ) is greater than zero,  $1 \le LZ \le NZ2$ , and for either a user specified number of  $X_2$  - coordinate locations (see NYREAD) or for a specified number of boundary locations (see NBCRD).

Namelist or Variable name

Description

\$BOUND

Initial Flow Field Setup

LZREAD(LZ)

Input sentinel for X<sub>3</sub> - grid point number LZ.

LZREAD = 0. No input will be read for this LZ

station; program sets up a default flow field

based on inlet profile data.

LZREAD = 1. Read boundary data into the array

AIE for this LZ station (see below).

LZREAD = 2. Read entire starting solution into

the array AIE for this LZ station (see below).

LZREAD = 3. Same as LZREAD = 2, except the

X<sub>3</sub> - velocity component will be a power law pro
file. Intended for pipe and channel flows.

NYREAD (LZ)

Number of  $X_2$  - coordinate locations for this LZ station at which namelist \$BCDATA will be read. Default is NUMDY + 2. Used only when LZREAD(LZ)  $\geq$  2. See INY2 description below.

NBCRD(LZ)

Number of boundary locations IBC (1 to 4) for this LZ station at which boundary data only will be read via namelist \$BCDATA. Default is 4. Used only when LZREAD(LZ) = 1. See INIBC description below.

**IBPOWR** 

Not used.

FNTURB, RADIUS, WINCL, XJCL, YJCL

Parameters used for defining optional power law velocity profile (LZREAD = 3). FNTURB is the power law exponent for the profile  $u_3/u_{\rm CL} = (1-\frac{r}{R})^{1/n}$ , where n = FNTURB, R = RADIUS,  $u_{\rm CL} = WINCL$ , and r is the radial coordinate measured from the location  $(x_1,x_2) = (XJCL, YJCL)$ .

Description

IVSØPT

Turbulent viscosity option used for computing initial  $\mu_{T}$  for two-equation turbulence model initialization.

IVS $\phi$ PT = 2. Code utilizes procedure described in Ref. 3.

IVS/PT = 3. Turbulent viscosities are supplied on input (see INVS below), thereby bypassing the programmed mixing length model formulation. Default is 2.

INVS

Turbulent viscosity may be loaded into AIE(LG, INVS) in namelist BCDATA when  $IVS \not DPT = 3$  option is being used. Default INVS = 7.

VISCIN

Nondimensional dynamic viscosity for laminar flow. Default is VISCIN = 1.0

NVINP

Number of variables to be read into the AIE array described below. Default NVINP = 7.

IEQINP(IVAR)

Array to relate the input variable number IVAR  $(1 \le IVAR \le NVINP)$  to the external equation number IEQ (Table II). The default values are given in Table VIII.

ISPRED

ISPRED = 0. Do not spread and decay inlet velocity profile.

ISPRED = 1. Spread and decay inlet velocity

ISPRED = 1. Spread and decay inlet velocity profile based on free jet similarity solution. Default is ISPRED = 1 if there is an inlet port.

DECAY

Velocity decay exponent for two-dimensional jets (DECAY = 0.5) and circular jets (DECAY = 1.0).

NJETS

Number of inlet port jets. Default NJETS = 1.

## Description

LXPC(IJ), LYPC(IJ)

The  $X_1$  and  $X_2$  grid point coordinates, respectively, for the port center of inlet port number IJ. Must be specified unless the actual physical coordinates XJZERO(IJ) and YJZERO(IJ) are specified instead.

XJZERO(IJ) YJZERO(IJ) The  $X_1$  and  $X_2$  physical coordinates, respectively, for the port center of inlet port number IJ.

LXSPRD(I,IJ) LYSPRD(I,IJ) LZSPRD(I,IJ)

The  $X_1$ ,  $X_2$ , and  $X_3$  grid point coordinates, respectively, that determine the points in the  $(X_1, X_3)$  plane and in the  $(X_2, X_3)$  plane to which the inlet jet will be spread. The indices I = 1 and I = 2 designate the lower and upper coordinates of the jet emerging from port number IJ.

# \$BCDATA

#### Flow field data input

AIE(LG, IVAR)

Nondimensional value of variable number IVAR (Table VIII) at grid point (LX,LY) for the current LZ station, where LG  $\equiv$  LX and LY is determined by INY1 and INY2 as described below. When boundary data is being read (LZREAD = 1), LG  $\equiv$  LY if INIBC = 1 or 2 and LG  $\equiv$  LX if INIBC = 3 or  $^{4}$ .

INYl

First LY (X<sub>2</sub> coordinate) grid point number for the data being loaded into the AIE array during the present \$BCDATA namelist read. Set by code.

INAS.

Last LY ( $X_2$  coordinate) grid point number for the data being loaded into the AIE array during the present \$BCDATA namelist read. Must be specified.

INIBC

IBC number (Fig. 3) for the boundary data being loaded into the AIE array during the present \$BCDATA namelist read. Used only when LZREAD(LZ) = 1.

NVINP, LEQINP(IVAR) If specified these values will override those set in namelist \$BOUND.

# Sample Input Decks

Several sample input decks are presented here including the control cards necessary for operation on the CDC 6600 with the Scope 3.4.4 or NOS/BE operating system. The first input deck (pp. 56 - 58) is the initial input stream used to begin the three-dimensional combustor simulation presented herein. The second input deck (p. 59) is a restart of a previous run from restart files saved on magnetic tape, and the third input deck (p. 60) is the restart deck required to initiate the nitric oxide (NOX) chemistry calculation from a previous run.

#### Description of Printed Output

The MINT combustor code provides detailed printed output so that a user can monitor the solution as it progresses in time, and examine the flow field at a user specified time-step-frequency. The initial phase of the printed output (pp. 61 - 77) contains primarily the namelist input described above. This is followed by the initial flow field print of which only a sample is shown on pp. 78 - 81, and then a sample periodic time step summary is shown on p. 82.

The first line of output is the heading "MINT COMBUSTION CODE", the second line will be either "INITIAL INPUT STREAM" for a run initiated from cards (IREST = 0) or "RESTART OPTION USED" for a run which is a restart of a previous run (IREST > 0). The next line of output appears only when a new restart dump is to be written (IREPUN > 0), however no internal positioning of restart files is performed by the code. The next line of output reads "DIML-DIMLO =", followed by the ten reference quantities:  $\text{Re}^{-1}$ ,  $p_{\text{D}}/\rho_{\text{D}}U_{\text{D}}^{2}$ ,  $p_{\text{D}}/\rho_{\text{D}}h_{\text{D}}$ ,  $(\text{RePr})^{-1}$ ,  $U_{\text{D}}^{2}/h_{\text{D}}$ ,  $\text{Re}^{-1}(U_{\text{D}}^{2}/h_{\text{D}})$ ,  $(\text{RePr})^{-1}(U_{\text{D}}^{2}/h_{\text{D}})$ , (ReSc)  $^{-1}$ , Bo  $^{-1}$ , and  $\sigma T_D^{l_l}/\sigma_{R_D}$ , respectively. The next line "T, P, H-TOTAL =", is followed by reference values for these quantities. Then namelist \$LIST2 is printed by subroutine BVIV, and contains the grid point indices shown in Figs. 3 and 4. If IGEOM < 0, the heading "\*\*\*\*GENERAL GEOMETRY COEFFI-CIENTS\*\*\*\*" is printed followed by a tabulation (for all  $X_1$  and  $X_3$ ) of the metric coefficients and their derivatives in the order h2, h1, h2-1, h1-1,  $\partial h_2/\partial n$ ,  $\partial h_2/\partial s$ ,  $\partial (h_1^{-1})/\partial n$ ,  $\partial (h_1^{-1})/\partial s$ . The three-point central difference operators  $(\delta_k, \delta_k^2)$  are then printed for directions k = 1, 2, 3. The namelist \$GRIDV, which contains the actual coordinates (X, Y, Z), grid spacing (DX, DY, DZ); and the Roberts' grid transformation factors (X1, X2, Y1, Y2, Z1, Z2), is printed by subroutine BVIV.

The remaining namelist variables have been described in the Input description subsection. The namelist \$BOUND is printed only if a new case is being started. Then a single line is printed containing the nondimensional time steps corresponding to the explicit-stability limits due to viscous terms, conduction terms, and the CFL limit. Subsequently, the namelists \$READ1, \$READ2, \$READ3, \$READ4, \$READ5, and \$CHEMD are printed in that order followed by a labeled "\*\*\*\* STARTING FLOW FIELD \*\*\*\*" print.

The three line summary output printed at the end of each time step is largely self-explanatory: VISC, STAB and CFL indicate the ratio of the actual time step DT to those explicit stability limit step sizes; SSTEST is the maximum relative change in any flow variable occurring at grid point LX, LY, LZ; RATIO is just SSTEST/SSEPS; DU, DV, DW, DR, DMF, DTN, DTKE, DTED, and DNO are the maximum relative changes in the variables u, v, w,  $\rho$ ,  $m_1$ , T, k,  $\epsilon$ , and  $m_{NO}$ , respectively. This is followed by the labeled summary output (NZ2 lines) from subroutine PRNTS.

The detailed printout obtained at a user specified time step increment is clearly labeled as follows: U-VEL, V-VEL, W-VEL, DENS ( $\rho$ ), ENTH (h or H), MFRAC1 ( $m_1$ ), MFPHI ( $\phi$ ) if chemistry is included, TKE (k), TDISS ( $\varepsilon$ ), PRESS ( $\rho$ -PNOM), TEMP, VISC ( $\mu_{\rm eff}$ ), DIV (indicates  $\nabla \cdot \vec{u}$ ), ZMIX ( $Z = W_m^{-1}$ ) and CHMIX ( $c_{\rm H} = c_p^{-1}$ ). The printer plots obtained at the end of a run are also labeled as above; TIME PLOTS, DIR-1 PLOTS, DIR-2 PLOTS and DIR-3 PLOTS are presented in that order.

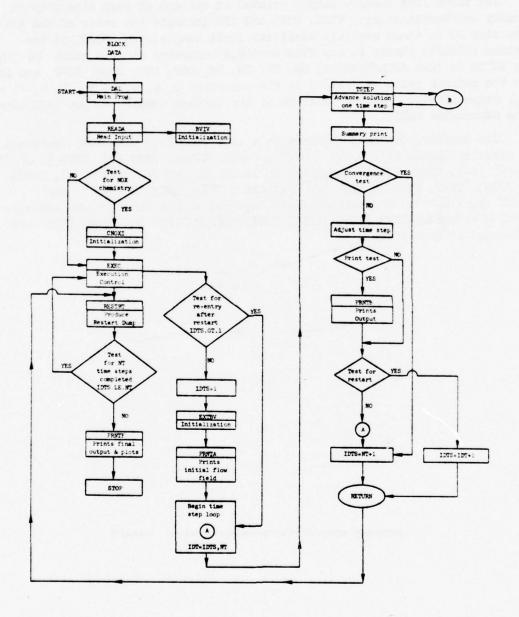


Figure 1. Flow diagram for MINT combustor code

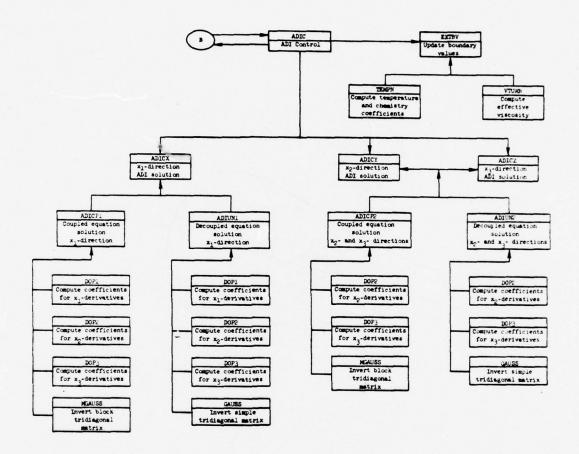


Figure 1(continued). Flow diagram for MINT combustor code

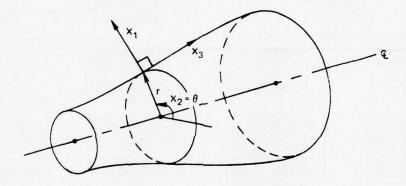


Figure 2. General axisymmetric combustor geometry.

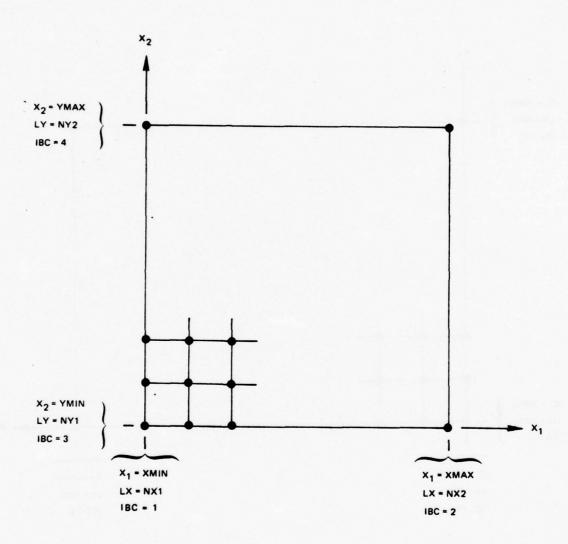


Figure 3. Computational grid notation:  $(X_1, X_2)$  plane.

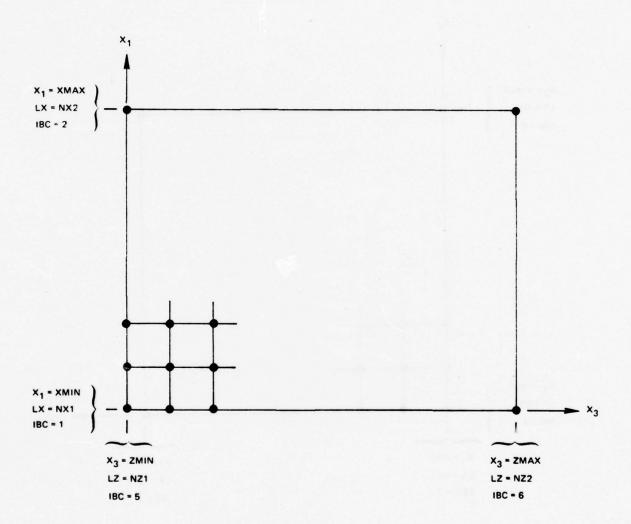


Figure 4. Computational grid notation:  $(X_1, X_3)$  plane.

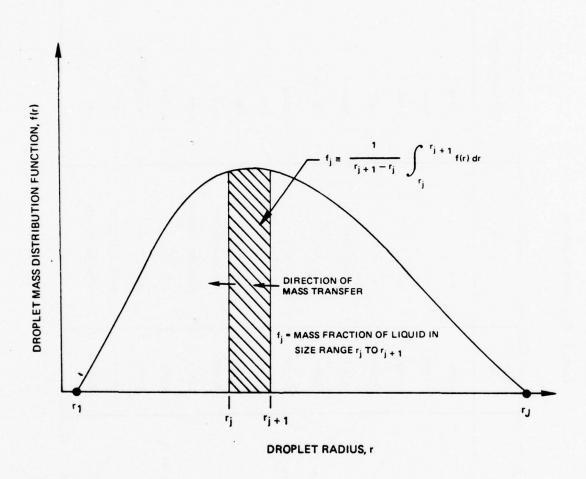


Figure 5. Schematic representation of particle fraction.

Table 1. References quantities

QUANTITY	FORTRAN	UNITS	DEFAULT VALUE
VELOCITY, UD	WREF	m/sec	NONE
LENGTH, L	CLENG	E	NONE
DENSITY, PD	DENSR	kg/m <sup>3</sup>	1.185
TEMPERATURE, TD	TREF	Уo	300.0
SPECIFIC HEAT, CpD	CPREF	joule/(kg- <sup>O</sup> K)	1004.8
DYNAMIC VISCOSITY, $\mu_D$	VISCR	kg/(m-sec)	1.816×10 <sup>-5</sup>
MOLECULAR WEIGHT, WD	WTREF	gm/mole	28.966
Pr.	PRNDL	NONDIMENSIONAL	0.73
Preff	PREFF	NONDIMENSIONAL	0.90
S	SCMDT	NONDIMENSIONAL	0.73
Scett	SCEFF	NONDIMENSIONAL	06:0
UNIVERSAL GAS CONSTANT, Rg	RGAS	joule /(mole- <sup>0</sup> K)	8.3143
PRESSURE, PD	PREF	pascal = $N/m^2$	10 <sup>3</sup> $ ho_{\rm D}^{\rm RgT_{\rm D}/W_{\rm D}}$
NOMINAL PRESSURE	PNOM	NONDIMENSONAL	1.0
SPECIFIC HEAT RATIO	GAMMA	NONDIMENSONAL	1.4

Table II. External equation and variable numbers

GOVERNING EQUATION	IEQ EXTERNAL EQUATION NUMBER	ASSOCIATED DEPENDENT VARIABLE	IVARNO (IEQ) DEFAULT VARIABLE NUMBER	ISOLVE (IEQ) SOLUTION MODE SENTINEL
X <sub>1</sub> – MOMENTUM	1	X <sub>1</sub> - VELOCITY COMPONENT, u	1	1
X <sub>2</sub> – MOMENTUM	2	X <sub>2</sub> - VELOCITY COMPONENT, v	2	1
X <sub>3</sub> - MOMENTUM	3	X <sub>3</sub> - VELOCITY COMPONENT, w	3	1
CONTINUITY	4	DENSITY, p	4	1
ENERGY	5 .	ENTHALPY, H OR h	5	1
FUEL SPECIES CONSERVATION	6	FUEL MASS FRACTION, m <sub>1</sub>	6	1
MIXTURE FRACTION CONSERVATION	7	MIXTURE FRACTION, Φ'	7	1
NO SPECIES CONSERVATION	8	NO MASS FRACTION, m <sub>NO</sub>	5	3
PARTICLE CONSERVATION, CLASS 1	9	PARTICLE FRACTION, f	10	2
PARTICLE CONSERVATION, CLASS 2	10	PARTICLE FRACTION, 12	11	2
PARTICLE CONSERVATION, CLASS 3	11	PARTICLE FRACTION, f <sub>3</sub>	12	2
PARTICLE CONSERVATION, CLASS 4	12	PARTICLE FRACTION, f4	13	2

TABLE II (continued). External equation and variable numbers

GOVERNING EQUATION	IEQ EXTERNAL EQUATION NUMBER	ASSOCIATED DEPENDENT VARIABLE	IVARNO (IEQ) DEFAULT VARIABLE NUMBER	ISOLVE (IEQ) SOLUTION MODE SENTINE
X <sub>1</sub> - RADIATION FLUX	13	X <sub>1</sub> – RADIATION FLUX FUNCTION, G <sub>1</sub>	14	2
X <sub>2</sub> - RADIATION FLUX	14	X <sub>2</sub> – RADIATION FLUX FUNCTION, G <sub>2</sub>	15	2
X3 - RADIATION FLUX	15	X <sub>3</sub> – RADIATION FLUX FUNCTION, G <sub>3</sub>	16	2
TURBULENCE KINETIC ENERGY	16	TURBULENCE KINETIC ENERGY, k	8	1
TURBULENCE KINETIC ENERGY DISSIPATION RATE	17	DISSIPATION RATE, $\epsilon$	9	1

Table III. Default values of ICPLD (IEQ, IADI)

IEQ	1	2	3
1	1	11	11
2	11	1	11
3	11	11	1
4	1	1	1
5	1	1	1
6	1	1	1
7	1	1	1
8	21	21	21
9	12	12	12
10	12	12	12
11	12	12	12
12	12	12	12
13	22	0	0
14	0	22	0
15	0	0	22
16	2	2	2
17	2	2	2

Table IV. Default values of IEQBC (IBC, IEQ)

IEQ IBC	1 334	2	3	4	5	6
1	1	1	2	2	5	3
2	2	4	1	1	5	3
3	2	4	2	2	5	3
4	2	4	2	2	4	4
5	2	2	2	2	7	3
6	2	2	2	2	. 5	3
7	2	2	2	2	5	3
8	2	2	2	2	5	3
9	2	2	2	2	5	3
10	2	2	2	2	5	3
11	2	2	2	2	5	3
12	2	2	2	2	5	3
13	2	4	0	0	0	0
14	0	0	2	2	0	0
15	0	0	0	0	4	4
16	2	2	2	2	5	3
17	2	4	2	2	5	3

# Table IV (continued). Default values of IBOUND (IBC) and ICONBC (IBC)

IBC	1	2	3	4	5	6
IBOUND (IBC)	2	4	2	2	1	1
ICONBC (IBC)	1	1	1	1	1	2

Table V. Chemical rate constants

k = A TN EXP (-B/RT).

1.0 z 0 0 REVERSE RATE 38640 48600 334 3.10×10<sup>13</sup> 1.55×10<sup>9</sup> 1.6×10<sup>14</sup> 4 0.1 z 0 0 FORWARD RATE 75400 6250 0.0 6.43×10<sup>9</sup> 1.36×10<sup>14</sup> 4.22×10<sup>13</sup> 4 N2+0=N0+N N + OH = NO + H N+02 = NO+0 REACTION

•UNITS ARE cm, cal, OK, g- mole., sec

Table VI. Chemical species identification

SPECIES NUMBER	CHEMICAL SYMBOL	MOLECULAR WEIGHT (gm/mole)
1_	H <sub>2</sub> O	18.0
2	co <sub>2</sub>	44.0
3	02	32.0
4	N <sub>2</sub>	28.0
5	A	39.94
6	н <sub>2</sub>	2.0
7	со	28.0
8	NO	30.0
9	ОН	17.0
10	н	1.0
11	0	16.0
12	CH <sub>4</sub>	16.0
13	ĈH₄ ô₂	16.0
14	ô <sub>2</sub>	32.0
15	NOT USED	

<sup>( )</sup> DENOTES PASSIVE (i.e., INERT) SPECIES FOR THE PARTIAL EQUILIBRIUM CALCULATION.

Table VII. Atomic stoichiometric coefficients BETA(IS,JE)

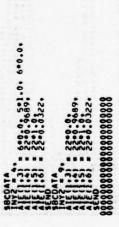
	JE	н	С	0	N	Α	ĈH₄	ô <sub>2</sub>
ıs		1	2	3	4	5	6	7
н <sub>2</sub> 0	1	2	0	1	0	0	0	0
co <sub>2</sub>	2	0	1	2	0	0	0	0
0,2	3	0	0	2	0	0	0	0
N <sub>2</sub>	4	0	0	0	2	0	0	0
A	5	0	0	0	0	1	0	0
н <sub>2</sub>	6	2	0	0	0	0	0	0
со	7	0	1	1	0	0	0	0
NO	8	0	0	1	1	0	0	0
он	9	1	0	1	0	0	0	0
н	10	1	0	0	0	0	0	0
0	11	0	0	1	0	0	0	0
CH <sub>4</sub>	12	4	1	0	0	0	0	0
с̂н <sub>4</sub>	13	0	0	0	0	0	1	0
ô <sub>2</sub>	14	0	0	0	0	0	0	1

<sup>( )</sup> DENOTES PASSIVE (i.e., INERT) SPECIES FOR THE PARTIAL EQUILIBRIUM CALCULATION

Table VIII. Default variable numbers for namelist input

IVAR	EXTERNAL EQUATION NUMBER IEQINP (IVAR)	ASSOCIATED INPUT VARIABLE
1	1	X1 - VELOCITY COMPONENT
2	2	X2 - VELOCITY COMPONENT
3	3	X3 - VELOCITY COMPONENT
4	4	STATIC PRESSURE
5	5	TEMPERATURE
6	6	FUEL MASS FRACTION
7	NONE	TURBULENT VISCOSITY
8-11	9–12	PARTICLE FRACTION, CLASSES 1-4
12	13	X1 - RADIATION FLUX COMPONENT
13	14	X2 - RADIATION FLUX COMPONENT
14	15	X3 - RADIATION FLUX COMPONENT

CONNECT: 1000-10750-CW200000-WTZ-51C5RAM
CONNECT: 1000-10750-CW200000-WTZ-51C5RAM
CONNECT: 1000-10750-CW200000-WTZ-51C5RAM
CONNECT: 1000-10750-CW200000-WTZ-51C5RAM
CONNECT: 1000-10750-CW200000-WTZ-51C5RAM
CONNECT: 1000-10750-CW20000-WTZ-51C5RAM
CONNECT: 1000-10750-CW2000-WTZ-51C5RAM
CONNECT: 1000-10750-CW2000-WTZ-51C5RAM
CONNECT: 1000-10750-CW200-WTZ-51C5RAM
CONNECT: 1000-10750-WTZ-51C5RAM
CONNECT: 1000-WTZ-51C5RAM
CONNECT:



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CONTRINCT

CONTRINCT
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CONTAINS OF CONTAINS OF CAME O
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. . . . . MINT COMBUSTION CODE

INITIAL INPUT STRFAM

RESTART GUTPUT UNIT NO. 10 POSITIONED AT RESTART DUMP NO. 1 0 PHYSICAL FILES SKIPPED

DIM! - DIMID = 1.6989E-05 1.1565E-01 2.8567E-01 2.3272E-05 2.4701E-02 4.1965E-07 5.7486E-07 2.3272E-05 0. T. P. H-TOTAL = 9.81251E-01 1.01213E-00 9.81251E-01

:

#LIST2

NX1 = 1:

NX2 = 17:

NY1 = 1:

NY2 = 9:

NX1 = 1:

LX1 = 2:

LX2 = 16:

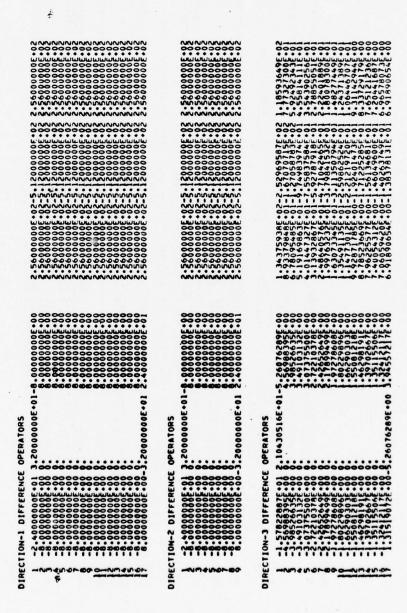
LY1 = 2:

LY2 = 8:

LY2 = 8:

LZ2 = 16:

SEND



<b>8GR 10v</b>			
		. 6875£-625E-015E-1025E-002E-1075E-003E-25E-003.3125E-003.315E-00.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0	
		0.0: .625E-01: .125E-00: .1875E-00: .25E-00: .3125E-00: .375E-00: .4375E-00: .5E-00: 0.0: 0.0: 0.0: 0.0: 0.0:	
		0.0. 10209022929283E.00. 21938489880412E.00. 35358558294606E.0050639452948436E.006794452114321E.00 2198125137546E.00. 10919128179E.01. 13333333333333335E.0155987880855697E.01. 18879415255819E.01 2198125137546E.01553197264176218E.0128821100068807E.0132464487313844E.0136206832280949E.01.	
*		.625E-01: .625E-	
6		.625E-01625E-01625E-01625E-01625E-01625E-01625E-01625E-01625E-01. 0.0. 0.0. 0.0. 0.0.	
20	•	10209002929283E.0011729486951128E.0013420068414194E.00265647520365391E.0017305068194774E.002656475203652E.0026647520362656475203626647520362664752036369144347721224.00369144347721224.00369144347721224.00369144347721224.00369144347721224.00369144347721224.00369144347721224.00369144347721224.003691443474721224.003691443474721224.003691443474747721224.003691443474747721224.0036914434747721224.003691443474747721224.003691443474747721224.0036914434747721224.0036914434747721224.0036914434747721224.0036914434747721224.0036914434747721224.00369144347721224.00369144347721224.00369144347721224.00369144347721224.00369144347721224.00369144347721224.00369144347721224.00369144347721224.00369144347721224.00369144347721224.00369144347721224.00369144347721224.00369144347721224.00369144347721224.00369144347721224.003691443477212244.00369144347721224.00369144347721224.003691443477212244.00369144347721224.00369144347721224.00369144347474747474.003691443474747474747474747474747474747474747	
¥		.16E-0216E-0216E-0216E-0216E-0216E-0216E-0216E-02 0.0. 0.0. 0.0. 0.0. 0.0. 0.0. 0	
12		0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,	
		*16E*02* .16E*02* .16E*02* .16E*02* .16E*02* .16E*02* .16E*02* .16E*02* .16E*02* 0.0* 0.0* 0.0* 0.0* 0.0*	
12		0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,	
	•	.105215257763 .0291397679075438E.014370532693308E.0159820626396435E.01614750997979678E.015544205955704 .014.75099979678E.01554425979555642E.0157023101225879E.012546242334457023101225879E.0125462423344583033814444081E.010.00.00.00.0.	
22	•	C.15782288666449E.0211605254886949E.028%503141703177E.01463355752078152E.0147057078886498E.01347958956449E.011479589564796E.011111974535777FE.01347958956479659093479589564796E.013479589564796E.013479589564796E.013479589564796E.013479589564796E.013479589564796E.013479589564796E.0134795897977E.01347958979797FE.0134795897977FE.01347958979797FE.01347958979777FE.01347958979777FE.01347958979777FE.01347958979777FE.01347958979777FE.01347958979777FE.01347958979777FE.013479589797777FE.013479589797777FE.013479589797777FE.013479589797777FE.013479589797777FE.013479589797777FE.013479589797777FE.013479589797777FE.013479589797777FE.013479589797777FE.013479589797777FE.013479589797777FE.013479589797777FE.013479589797777FE.013479589797777FE.013479589797777FE.013479589797777FE.0134795897977777FE.0134795897977777FE.0134795897977777FE.0134795897977777FE.01347958979777777FE.01347958977777FE.0134795897977777777777777777777777777777777	
SEND			

STABILITY LIMITS (VISC. COND. CFL) . 4.84105E+01 2.52426E+01 9.17365E-03

\$PE 401 | PE 5T = -1. | IRE PUN = 2. | MINPD = 0. | INTAPE = 9. | IOTAPE = 10. | MF UV = 1.

67

LYSPLT
LYSPLT
CLENG
NEWGRD
IDMPX
INTINE
NATINE

= .58862087279735E+05. = .73E+00. . .24996120547945E-01. .64179234508504E+03. . .10350393594214E-06. . .34523234136574E.02. .24852275229127E .00. \* .66666667E .00. . 102992E . 07. - .10048E-04. .28966E . 02. . .83143E+01, . 1025E . 04. . .1816E-04. .1905E-01. \* .1595E + 03+ - .3518E · 00. .9995E.00. .9689E .00. . .146.01. . .73E .00. .16.31. . .9E.00. . .SE + 00. \* .9E .00 \* .11.31. . . .SE .00. 0.0 LAMFLO SREADS SOUND 804.72 VISCR CLENG VISCL PRNOL SCHOT DENSA WTREF GAMMA POROP PREFF DAREF REAS SCEFF CPREF DREF PNOM HREF HREF ZREF TREF

AVISC3 = .5E.00,
IM57A6 = 0,
IMFDIF = 2,
IMVISC = 3,
VPLO = .2E.01,
VPHI = .1E.03,
CLANDA = .8E.01,
CVK = .8E.01,
CVK = .4E.00,
CLUI = .2E.01,
CVK = .4E.00,
CLUI = .2E.01,
CVK = .9E.01,
CYRBU = .9E.01,
SIGK = .1E.01,
SIGK =

```
. 1. 2. 3. 4. 5. 6. 7. 5. 10. 11. 12. 13. 14. 15. 16. 8. 9.
                = 1. 2. 3. 4. 5. 6. 7. 16. 17. 0. 0. 0. 0. 0. 0. 0. 0. 0.
                               . 1. 1. 1. 1. 1. 1. 1. 3. 2. 2. 2. 2. 2. 2. 2. 1. 1.
                                                                                                                                                                              ::
                                                                                                                                                               . 10.
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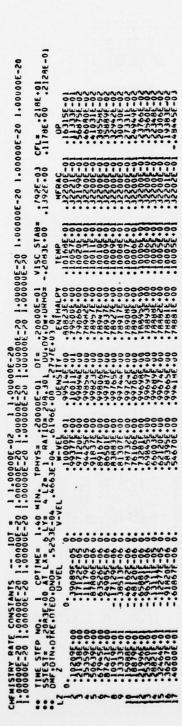
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